



Co-Optimization of
Fuels & Engines

Heavy-Duty Mixing-Controlled Compression Ignition (MCCI): MCCI and Ducted Fuel Injection, Part 1

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June 12, 2019
Project ID: FT077



FY19 Vehicle Technologies Office Annual Merit Review

better fuels | better vehicles | sooner

U.S. DEPARTMENT OF
ENERGY

Energy Efficiency &
Renewable Energy

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Overview



Projects

Abbrev.	Description
DFI	Fuel effects on mixing-controlled compression-ignition (MCCI) combustion & ducted fuel injection (DFI): Mueller
Soot	Soot-formation processes under MCCI combustion: Skeen

Timeline

Project	Start	End	% Complete
DFI	Oct. 1, 2018	Sept. 30, 2021	18%
Soot	Dec. 1, 2018	Sept. 30, 2021	12%

Barriers*

- Need improved combustion modes & understanding of fuel effects thereon
 - MCCI (a.k.a. clean-diesel) combustion
 - > Elevated nitrogen oxides and particulate emissions
 - > High costs of engine & aftertreatment systems
 - Sprays
 - > Lack of high-quality, fundamental data
 - > Inadequate predictive modeling capabilities

*from https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf, <https://www.energy.gov/eere/vehicles/advanced-combustion-strategies>, <https://energy.gov/eere/vehicles/us-drive-partnership-plan-roadmaps-and-accomplishments>

Budget

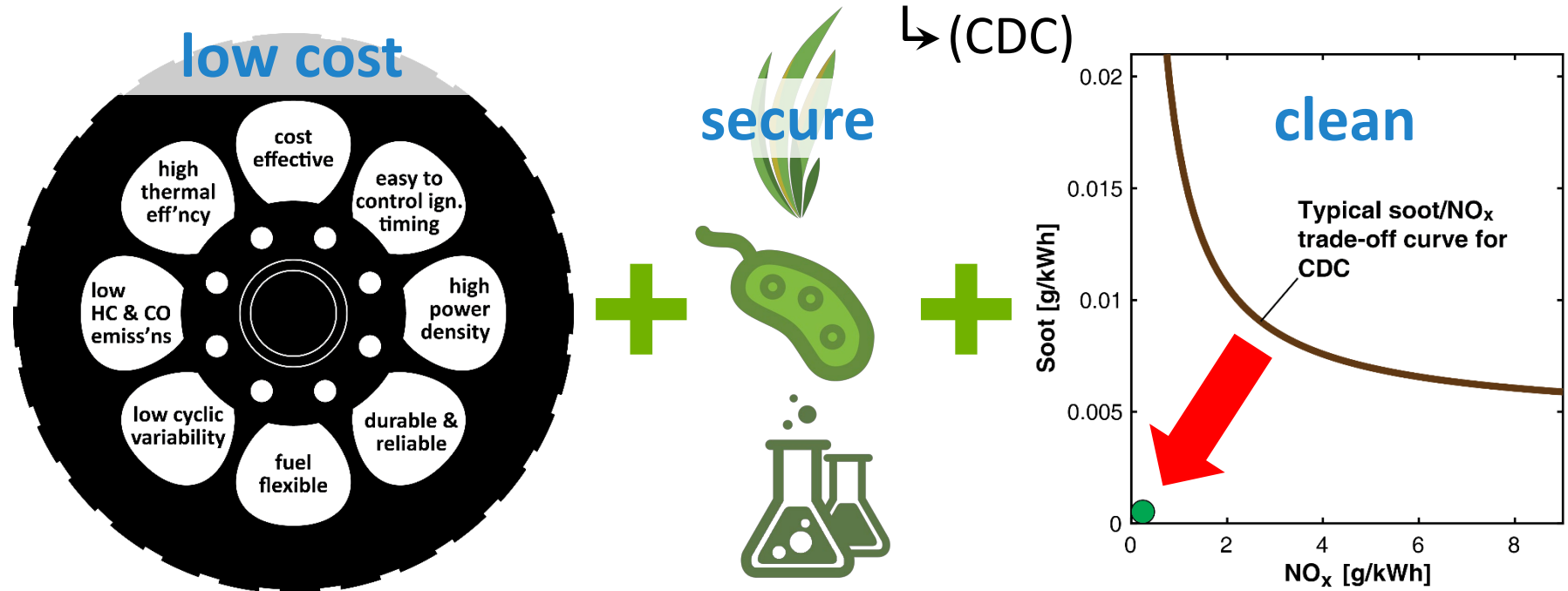
Project	FY18 [\$k]	FY19 [\$k]
DFI	540	640
Soot	0	180

Acronym & other definitions are listed in black, italic text at the bottom of this & subsequent slides: FY = fiscal year, runs October 1 – September 30; \$k = \$1000. **Next slide:** HC = hydrocarbon; CO = carbon monoxide



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Maintain the desirable attributes of conventional diesel combustion...

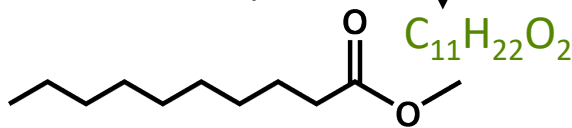


...while harnessing synergies with sustainable, home-grown fuels
...with 10X – 100X lower soot & nitrogen oxides (NO_x) emissions

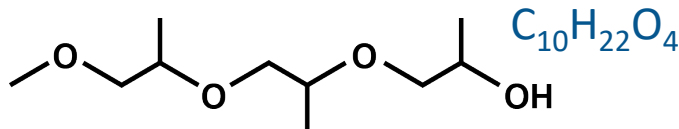
Employ unique experimental capabilities to develop an enhanced understanding of ducted fuel injection (DFI) & spray processes.

Using the only DFI engine in the world, **determine whether fuel oxygenation enhances DFI soot reduction.**

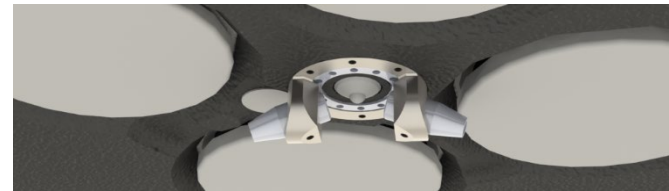
- **CFB** = No. 2 emissions certification diesel fuel, < 15 parts per million sulfur
- **MD25** = 25 vol% methyl decanoate (biodiesel-like ester) in CFB



- **T25** = 25 vol% tri-propylene glycol mono-methyl ether in CFB



Two dilution levels (16 & 21 mol% O_2),
start of comb. @ TDC, const. inj. energy.



2 × 108 μm × 140° tip with 2 ducts: 2 mm inner diam., 12 mm long, 3 mm from orifice exit

- Quantitative soot measurements in high-pressure pyrolyzing sprays:
decouple soot in sprays from ignition/lift-off characteristics of fuel (simplifies chemistry)
- Pilot-ignited jets/sprays:
unique potential to decouple ignition/lift-off properties from soot under oxidizing conditions

vol% = volume percentage; mol% = molar percentage; O_2 = oxygen; TDC = top dead center (i.e., piston @ top of stroke)

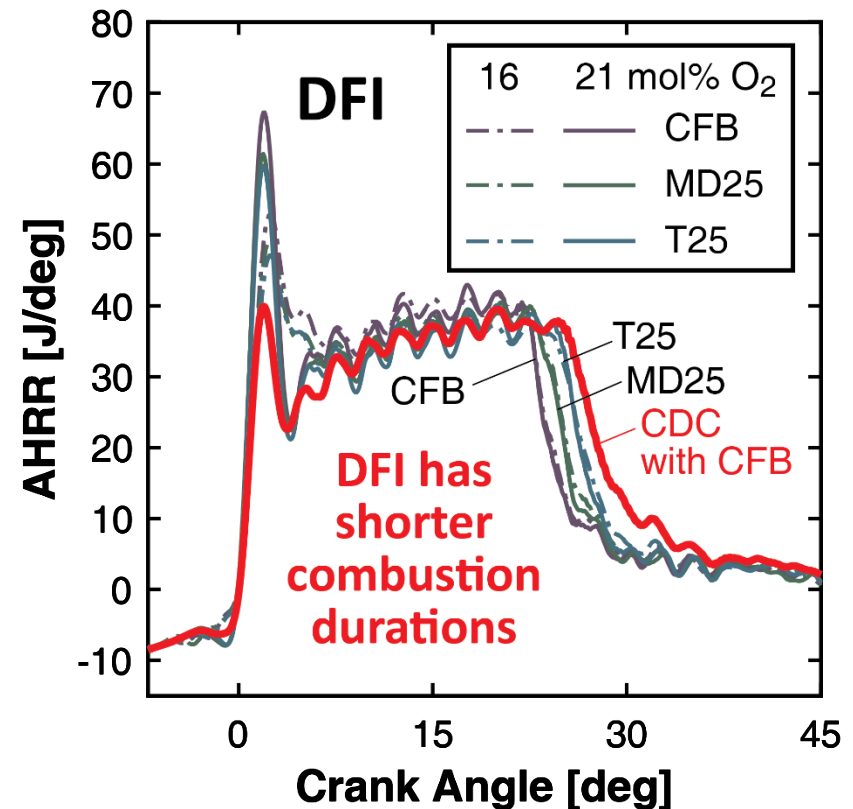
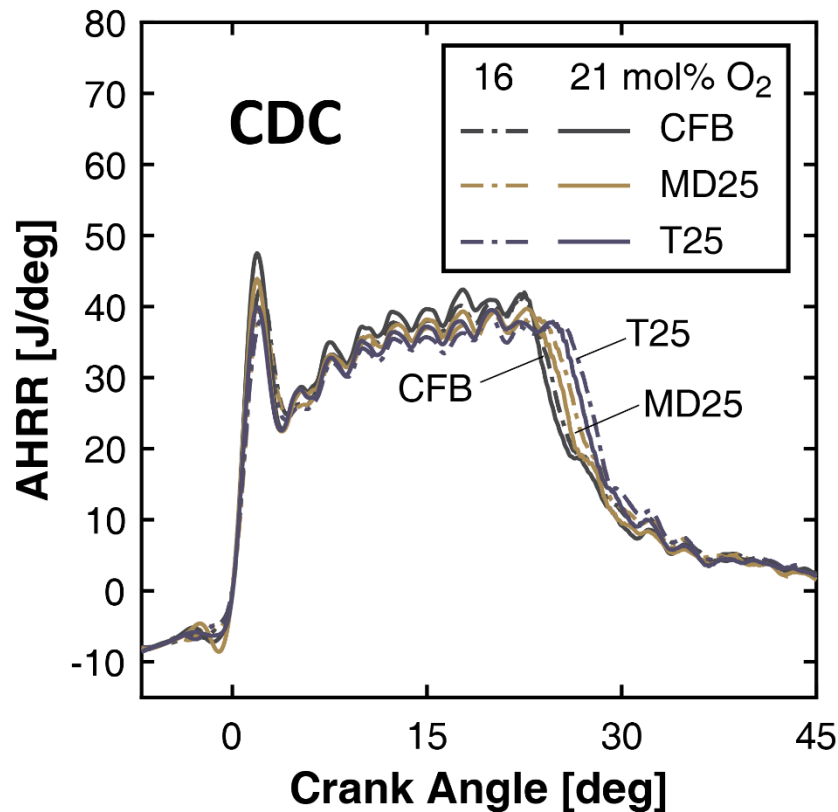


FY19 Milestones

Mo/Yr	Proj.	Description of Milestone or Go/No-Go Decision	Status
Dec. '18	DFI	Demonstrate successful quantitation of in-cyl. soot distrib'n via existing vertical laser-induced incandescence (VLII) data	Done
Mar. '19	DFI	Complete <u>CDC</u> engine testing of two oxygenated fuels & baseline diesel fuel at baseline conditions	Done
Mar. '19	DFI	Complete <u>DFI</u> engine testing of two oxygenated fuels & baseline diesel fuel at baseline conditions	Done
Sep. '19	DFI	Go/no-go: Does fuel oxygenation affect DFI?	On track
Mar. '19	Soot	Develop new experimental capability to decouple lift-off/ignition properties from soot in turbulent jets and sprays <ul style="list-style-type: none">• Q2: proof-of-concept in atmospheric pressure jets• Q3: go/no-go for implementation at high pressure	On track
Jul. '19	Soot	Piloted-ignition gas jet soot experiments with six fuels	On track
Sep. '19	Soot	Evaluate effects of aromatic dopants in n-dodecane on sooting propensity in pyrolyzing sprays	On track

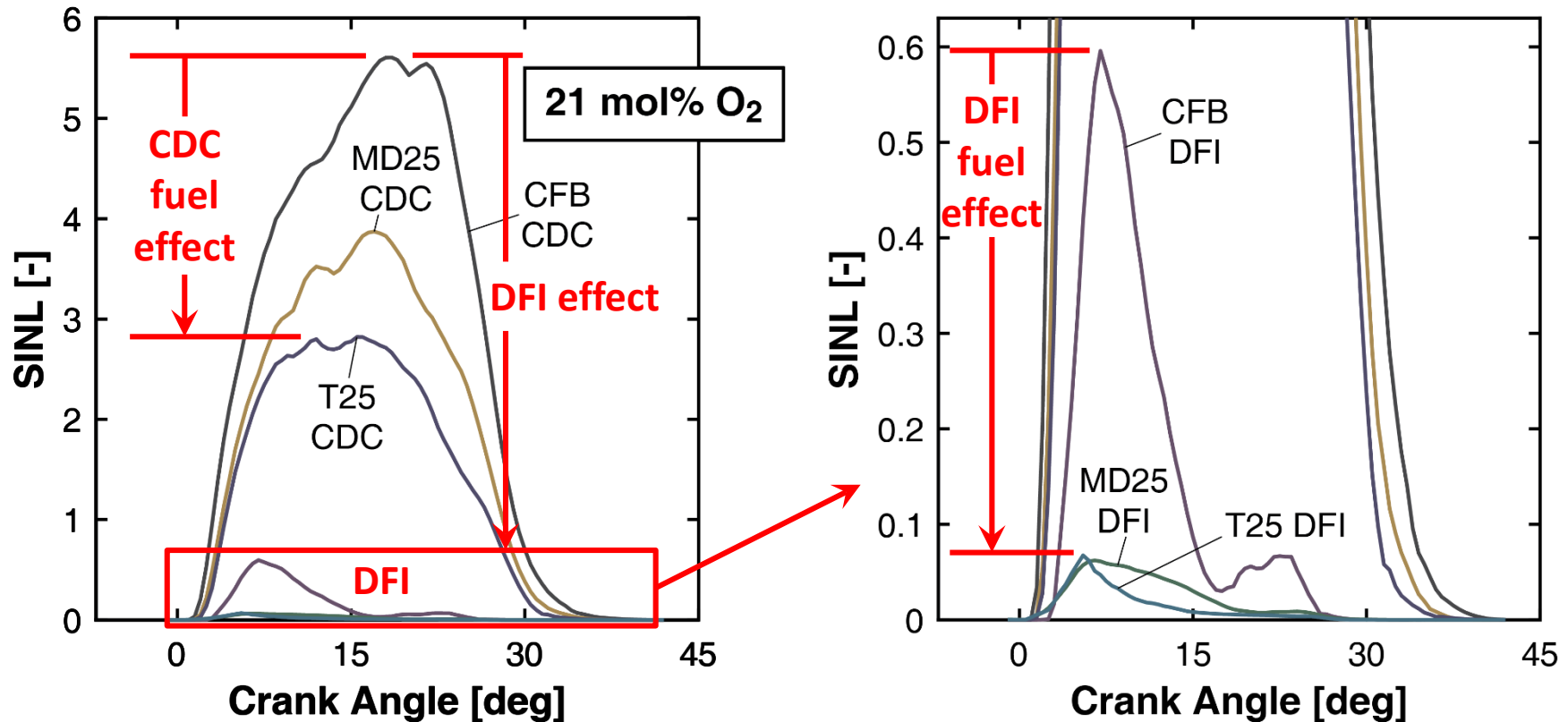
Q2 = second quarter of fiscal year, i.e., January-March; Q3 = third quarter of fiscal year, i.e., April-June

DFI with two ducts has been successfully tested in the optical engine with diesel fuel & two oxygenates.



- DFI exhibits apparent heat-release rates (AHRR) that are similar in shape & features to those for CDC
 - DFI has larger premixed burns & shorter combustion durations
- AHRRs are slightly longer for the oxygenated blends

Both fuel oxygenation & DFI are effective at curtailing incandescence from in-cylinder soot.

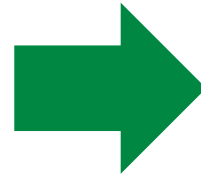
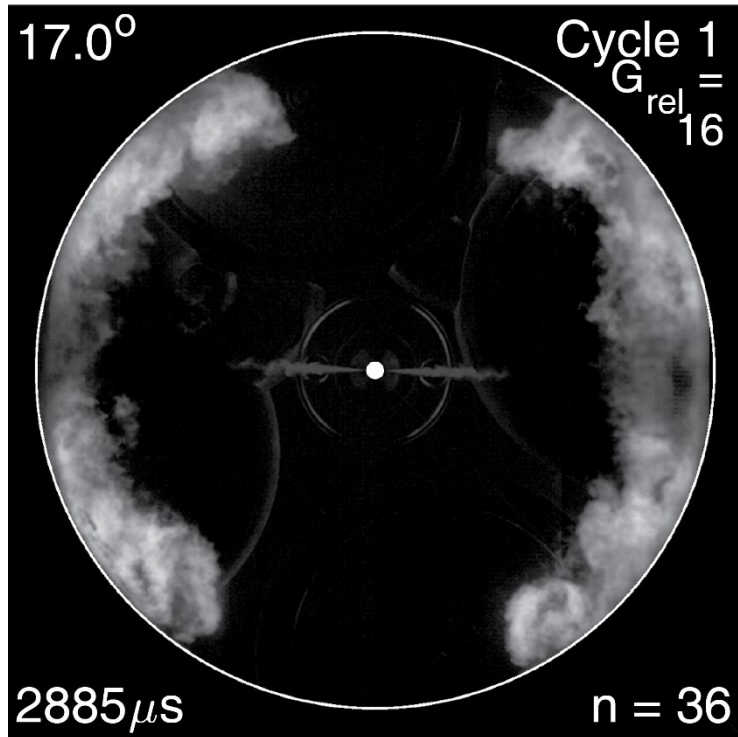


- Changing from CDC to DFI lowers spatially integrated natural luminosity (SINL) more than adding 25 vol% of either oxygenate
 - SINL is an indicator of hot, in-cylinder soot
- The fuel effect is larger for DFI than for CDC (on % basis)

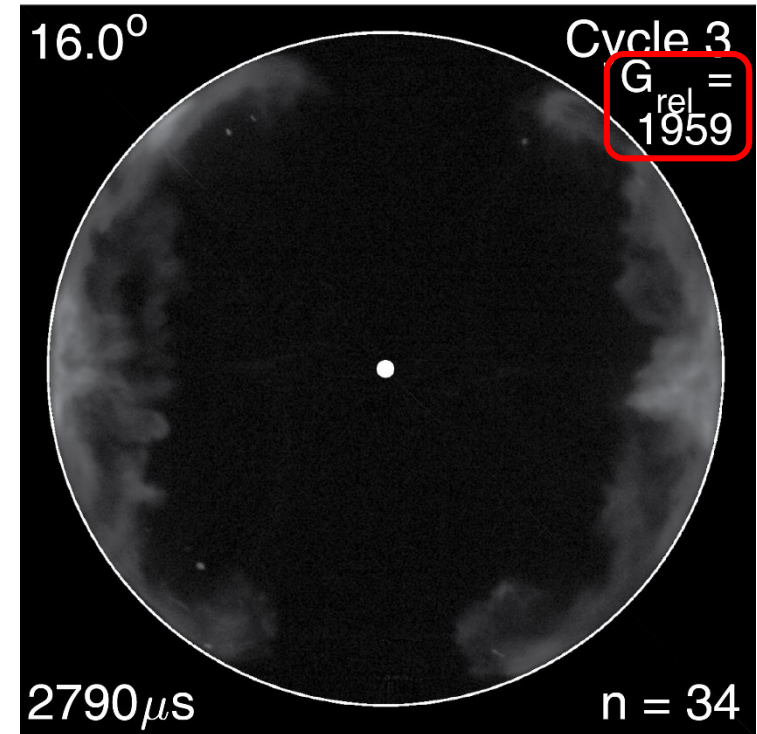
Fuel oxygenation & DFI together can curtail SINL by ~100X, effectively preventing soot formation.



CFB CDC



T25 DFI



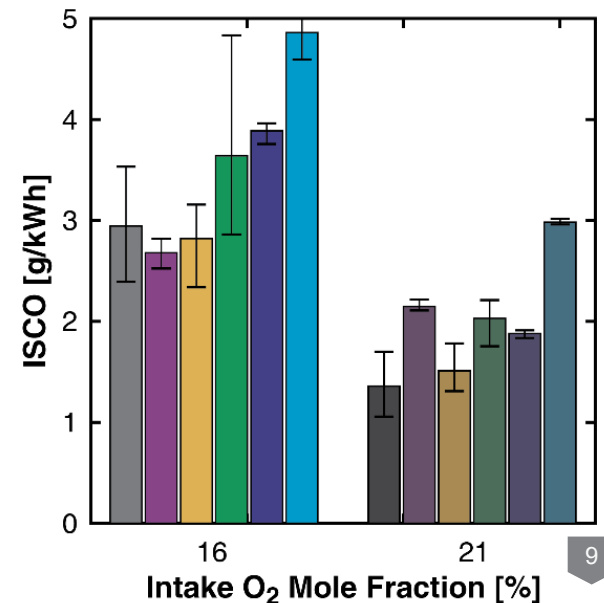
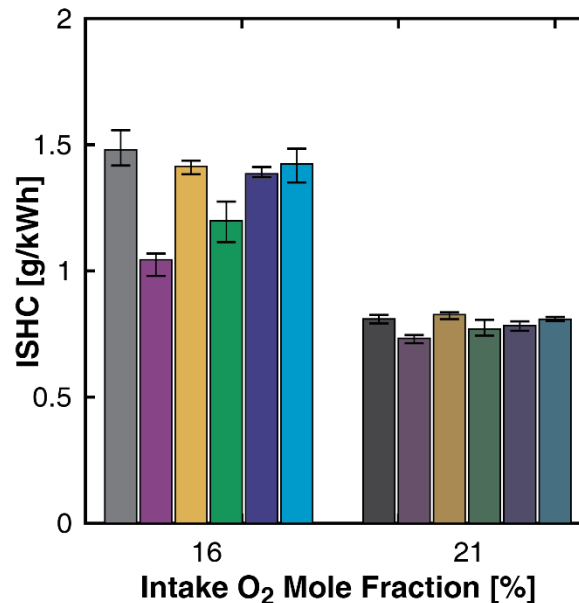
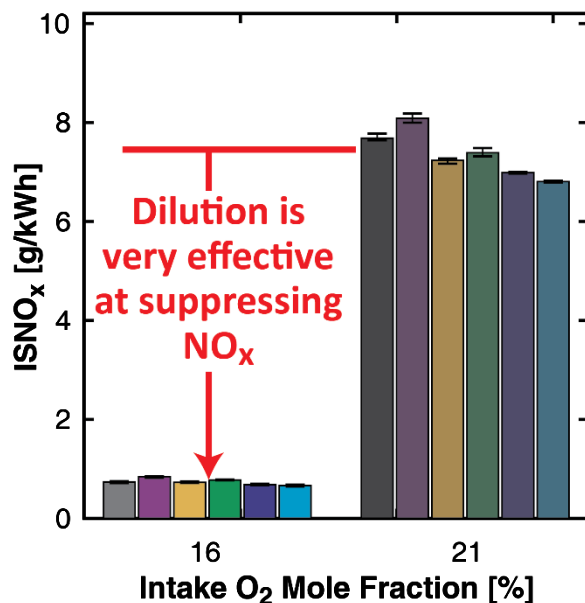
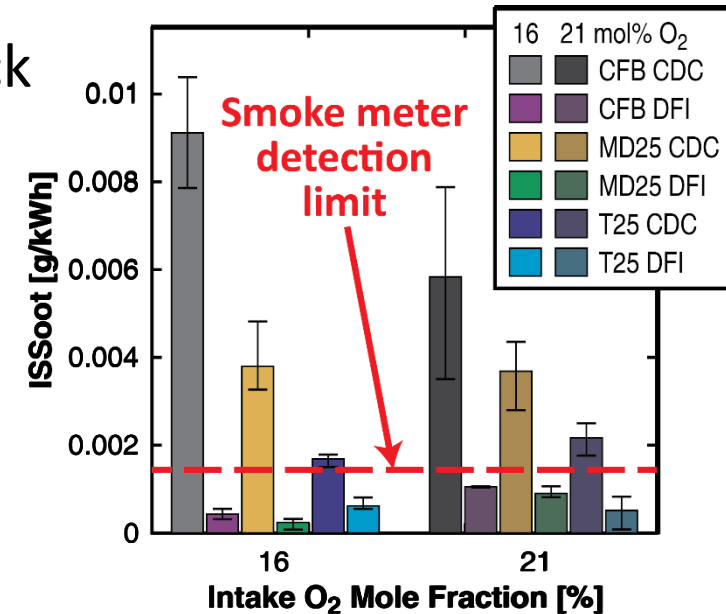
Status quo:
Significant in-cyl. & engine-out soot

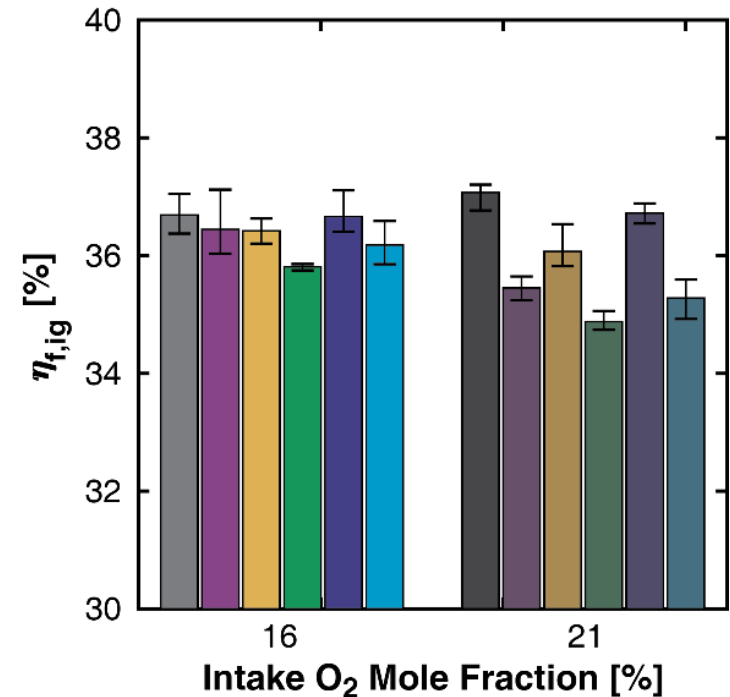
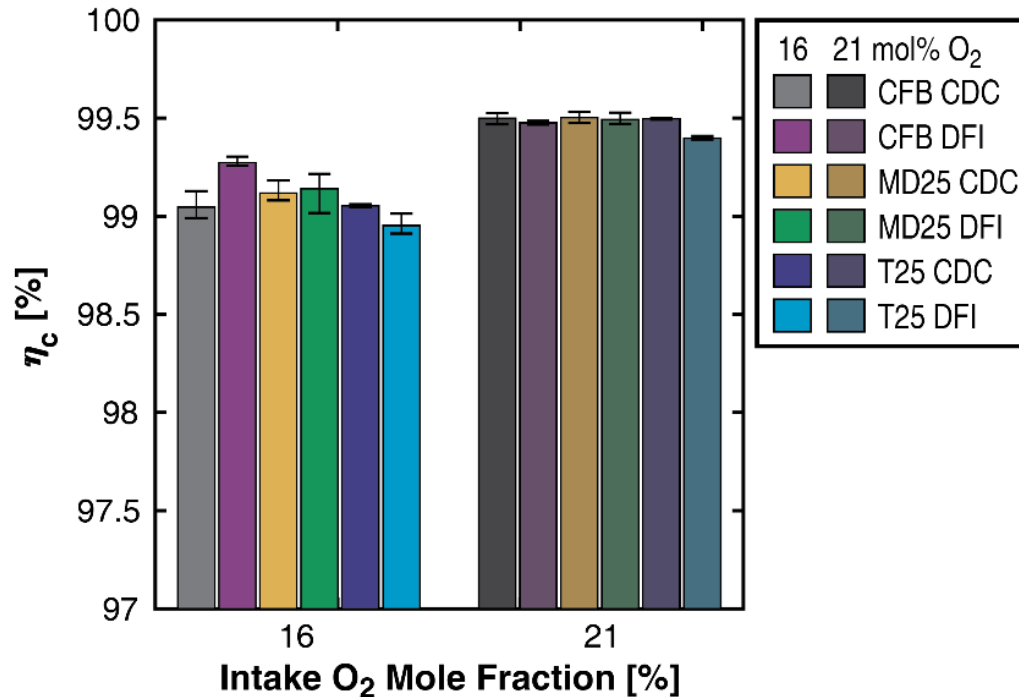
Leaner lifted-flame combustion:
“Zero” in-cylinder soot

Transition: Still make soot within the cylinder, but it is fully oxidized
before the exhaust valves open → “zero” engine-out soot



- Indicated specific (IS) soot emissions track with observed SINL trends
 - Soot for DFI is below detection limit
- $ISNO_x$ typically \downarrow with fuel oxygenation
- ISHC is typically maintained or improved via oxygenation & DFI
- ISCO typically \uparrow with oxygenation & DFI



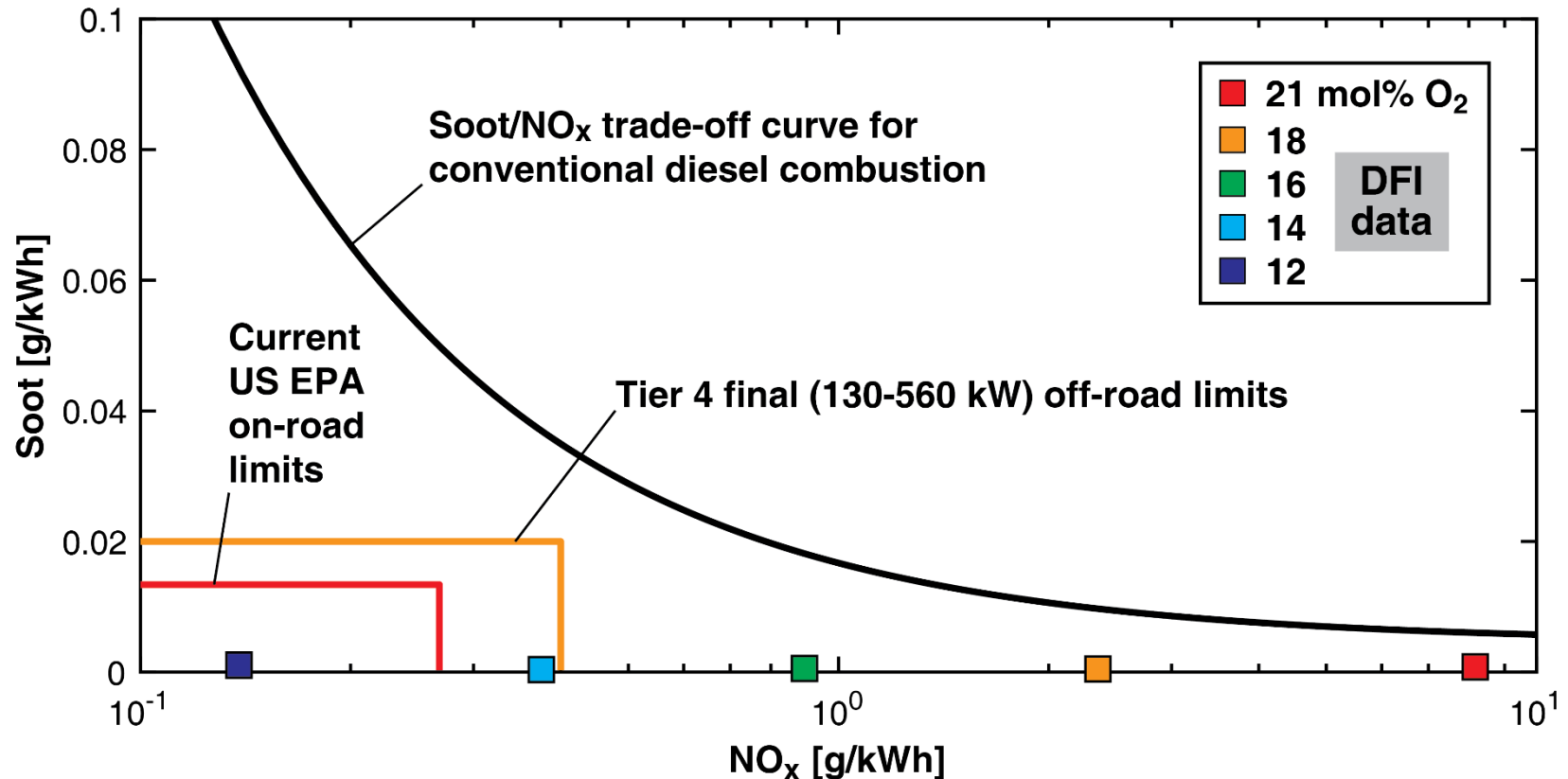


- Combustion eff's (η_c) are typ. $\geq 99\%$, may \uparrow or \downarrow with fuel & DFI
- Gross indicated fuel-conversion efficiencies ($\eta_{f,ig}$) typically \downarrow with fuel oxygenation ($< 1.0\%$ abs.) & with DFI ($< 1.6\%$ abs.)
 - Likely at least partially due to \uparrow injection duration & \uparrow heat transfer to piston bowl wall, respectively

With soot no longer a problem, intake-charge dilution can be used for cost-effective NO_x control.



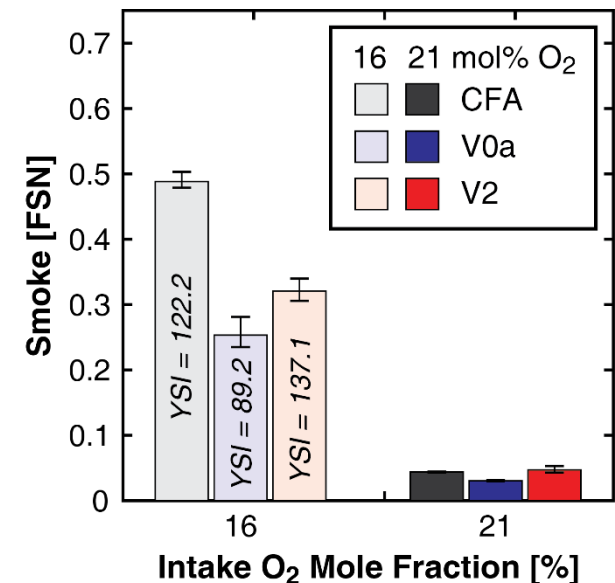
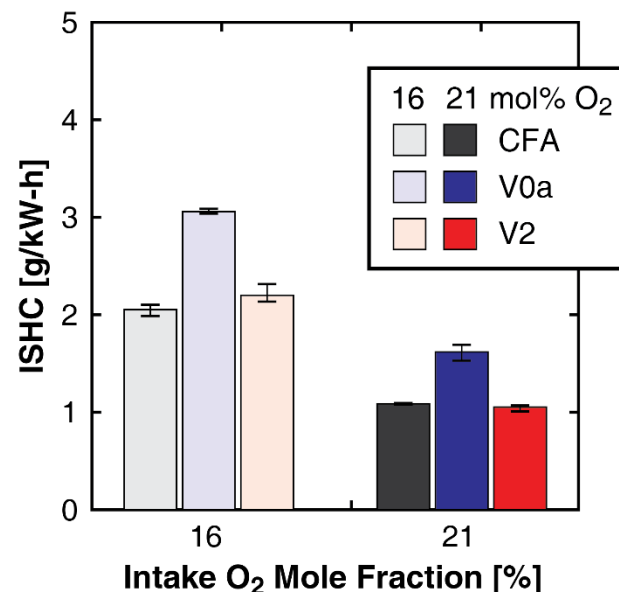
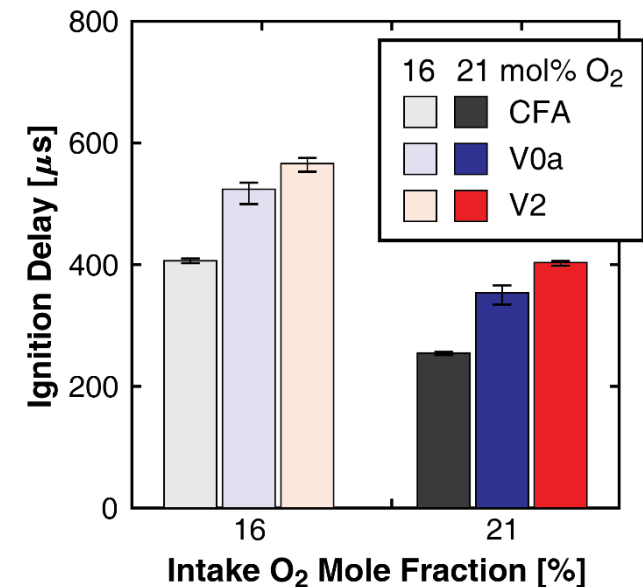
- DFI breaks the long-standing soot/NO_x trade-off with dilution, enabling simultaneous reductions in engine-out soot & NO_x

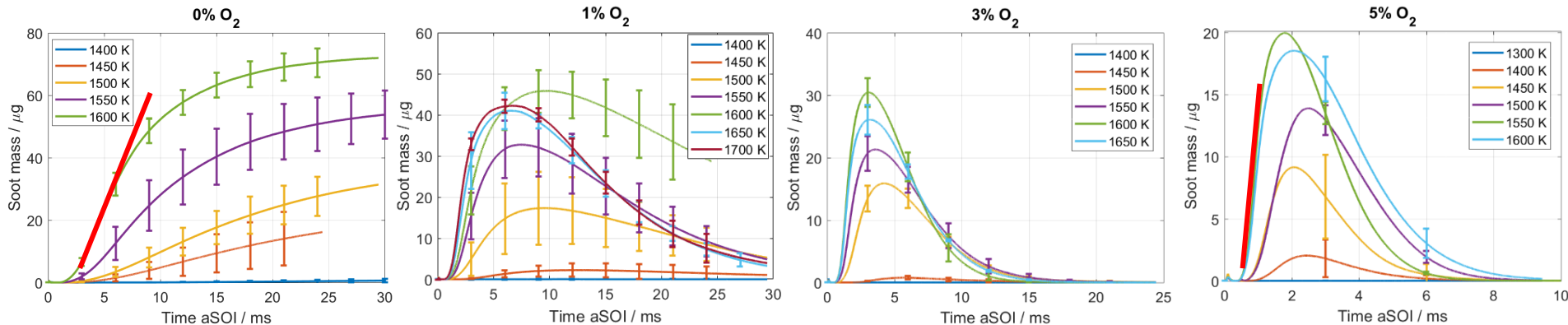


- Orders of magnitude lower: soot with DFI, NO_x with dilution

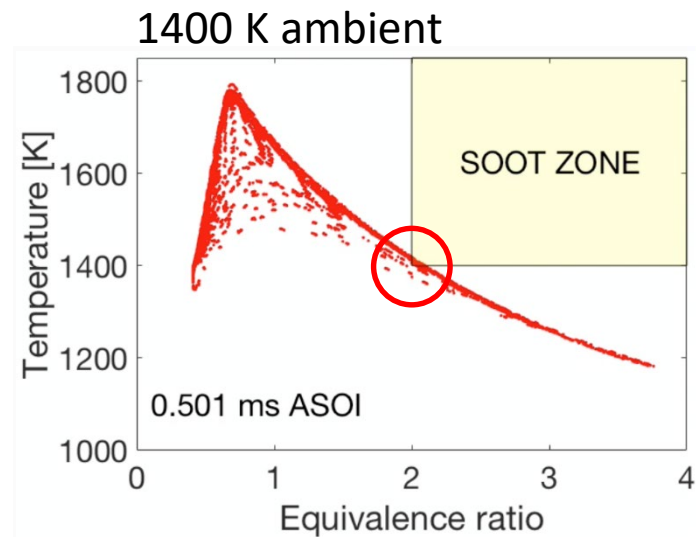
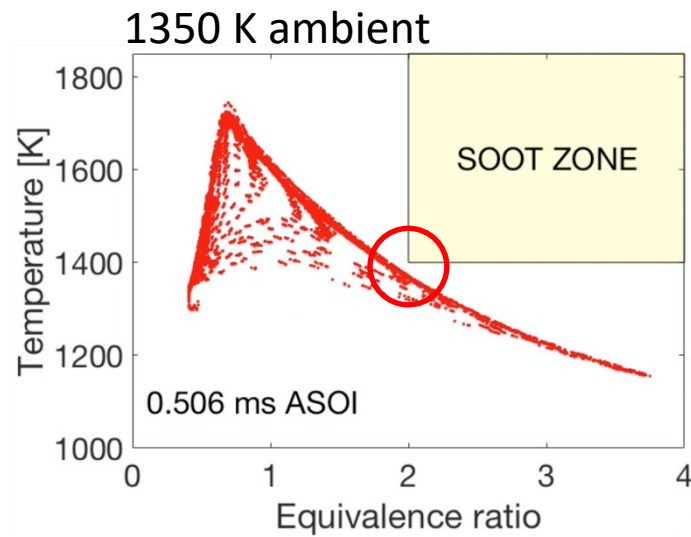


- Tested target fuel (CFA), simplest surrogate (V0a), & most-complex surrogate (V2)
 - From Coordinating Research Council Project AVFL-18/18a
- Ignition delays were different, despite fuel derived cetane numbers being matched
- Smoke emissions: Not explained by yield sooting index (YSI) or ign. delay diff's alone
- HC emissions:
 - ~50% higher for V0a than for V2 or CFA
- Why does V2 provide a better match than V0a?





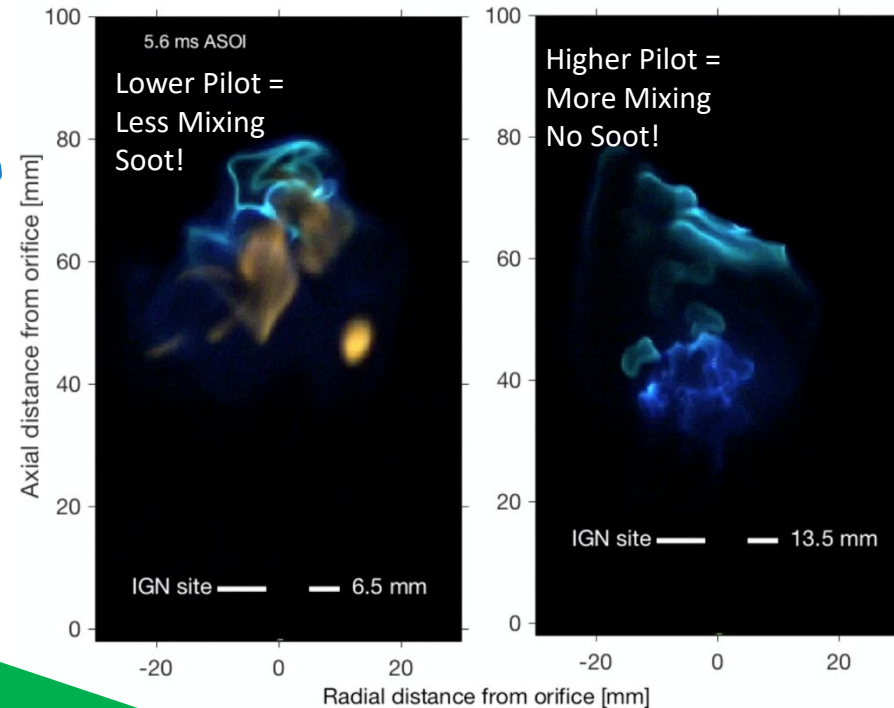
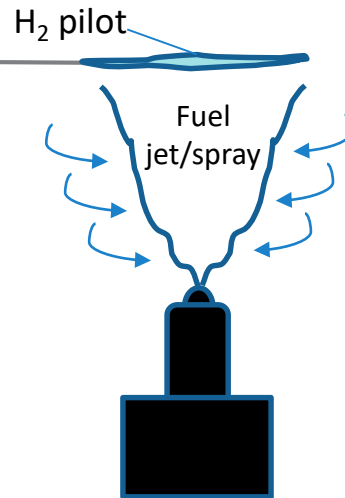
- 1400-1450 K critical temperature demonstrated for 0% O_2
- Addition of oxygen does not reduce critical temperature barrier to soot inception but greatly accelerates soot formation once it begins
- Computational Fluid Dynamics (CFD) simulations at 5% O_2 and 1400 K ambient: sufficient heat release occurs in equivalence ratio $\phi > 2$ regions to surpass critical soot formation temperature



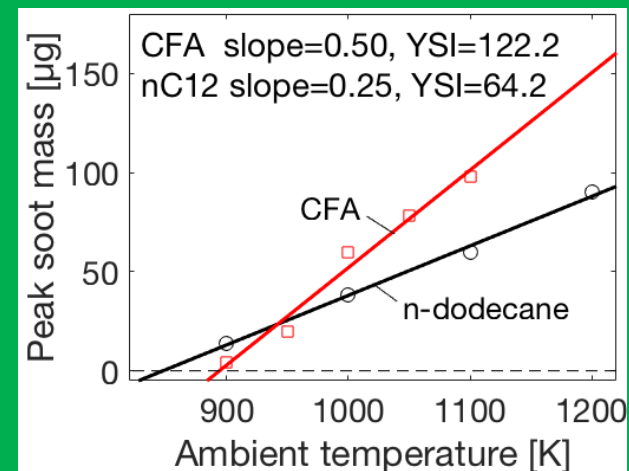
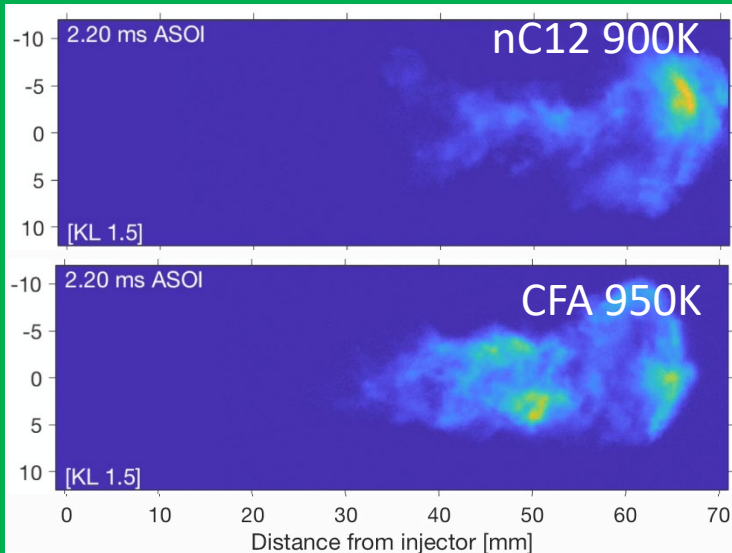
(1) New concept to decouple CN & soot (2) Correlation observed between YSI & quantitative soot in sprays



- Proof-of-concept with ethylene gas jet injected using single-hole GDI injector
- Hydrogen micro-jet pilot ignition occurs at user specified height above orifice
- Extent of mixing governed by pilot height



CN = cetane number; YSI = yield sooting index; GDI = gasoline direct injection; nC12 = n-dodecane; CFA = commercial No. 2 diesel fuel



Responses to Previous Year's Reviewers' Comments



DFI

Most feedback was positive; e.g., this is “some of the most interesting and potentially breakthrough work in the DOE portfolio,” and “continue strong support of this DFI project and consider increasing the budget and scope.”

- *Response: We are grateful to the reviewers for their encouraging comments!*

“Trying to pack five projects into one review is too much.”

- *Response: This year, the line-up was changed; this presentation only covers two projects.*

The DFI project “is quite interesting,” but the reviewer was “not sure how to implement it on ICEs. Hopefully, the PI can come up with a solution.”

- *Response: This year we have gained a good deal of experience with baseline DFI hardware & fuel effects. We are working closely with industry partners & other Co-Optima teams to move DFI closer to production as quickly as possible. See also DOE Off-Road Project ACE131.*

DFI “did not seem at all related to Co-Optima.” (Due to lack of a fuel-effects component?)

- *Response: In contrast to FY18, the Co-Optima DFI efforts in FY19 only concern fuel effects.*

There seems to be “too much focus on DFI in the future plans. If understanding how to co-develop a mixing controlled combustion system with new fuels is wanted, the reviewer suggested starting without something like DFI and fully understanding how the fuels interact with more conventional combustion system design variables.”

- *Response: A significant body of literature already exists in the area of MCCI fuel effects without DFI. DFI shows potential to be a feasible path to dramatically cleaner engines & sustainable fuels, & this justifies a future research approach that focuses on DFI.*

Soot

No reviewer comments – this project was a new start in FY19.



DFI	<ul style="list-style-type: none">• NREL (McCormick, Vardon): Selecting current & future oxygenated fuels & properties for facilitating optimal DFI performance• LBNL (George): Desired fuels & fuel properties for MCCI & DFI• ANL (Som): Accurate simulation of fuel effects on DFI• LLNL (McNenly): VLII signal quantification• LLNL (Pitz): Diesel surrogate formulation• Coordinating Research Council: Diesel surrogate fuels• Caterpillar: DFI & Technology Commercialization Fund CRADAs• Ford: DFI & Technology Commercialization Fund CRADAs
Soot	<ul style="list-style-type: none">• LLNL (Pitz): Kinetic model development/testing, reaction analysis• Caterpillar: Injector hardware, Converge simulations• IFPEN: Converge simulations, soot model evaluation/development• CMT: Converge simulations, soot model evaluation/development• NREL (Vardon): Selecting high cetane number oxygenated fuels for minimal soot formation in MCCI operation (SNL vessel experiments)• SNL/JBEI (Davis): Ignition and soot characterization of algae-derived fuels

NREL = National Renewable Energy Lab.; LBNL = Lawrence Berkeley National Lab.; ANL = Argonne National Lab.; LLNL = Lawrence Livermore National Lab.; CRADA = Cooperative Research and Development Agreement; IFPEN = Institut Francais du Petrol Energies Nouvelles, France; CMT = CMT-Motores Térmicos, Universitat Politècnica de València, Spain; SNL = Sandia National Labs; JBEI = Joint BioEnergy Institute.

Remaining Challenges and Barriers



DFI	<p>What are the effects of fundamental fuel-property changes on DFI?</p> <ul style="list-style-type: none">• <i>To what extent does higher ignition quality help or hurt?</i>• <i>How does fuel-oxygenation level map to engine-out soot emissions?</i>• <i>How important is oxygenate molecular structure?</i>• <i>How important are other fuel properties: volatility, density, compositional characteristics, yield sooting index, lower heating value, viscosity, ...?</i>• <i>How important are interactions among the above parameters?</i> <p>Can DFI benefits be realized over an acceptable range of engine loads & speeds?</p> <p>Will DFI be durable to deposit build-up and/or thermal/mechanical stresses?</p> <ul style="list-style-type: none">• <i>Can fuel-property changes mitigate any of these potential issues?</i> <p>What are the underlying reasons for the observed performance diff's among MCCI surrogate fuels having properties that are well-matched to the target fuel?</p>
Soot	<ul style="list-style-type: none">• Implementation of piloted-ignition spray setup into high-pressure facility• Aromatic dopant effects on ignition/lift-off too severe• Quantitative mixing measurements may be necessary to achieve greatest benefit from pyrolysis experiments• Additional soot data req'd to develop empirical model for MCCI soot metric• CFD simul'ns must overcome inability to capture soot under pyrolysis cond's



Proposed Future Research

*Any proposed future work
is subject to change based
on funding levels.*



DFI (all FY20)	<p>Explore the effects of fundamental fuel-property changes on DFI:</p> <ul style="list-style-type: none">• Use ignition improver to study effects of varying ignition quality• Use two Co-Optima oxygenated fuels at different blend levels to study effects of oxygenation level & oxygenate molecular structure <p>Test remaining diesel surrogate blends in the optical engine to assess their performance, better understand fuel-property effects, and guide development of further surrogate improvements.</p>
Soot	<p>FY19</p> <ul style="list-style-type: none">• Piloted-ignition gas jet experiments with six fuels (Q4 milestone)• Development of piloted-ignition spray in high-pressure vessel• Pyrolyzing sprays of aromatic doped n-dodecane (1,2,3-ring species) (Q4 milestone) <p>FY20</p> <ul style="list-style-type: none">• Ignition/lift-off characterization of aromatic doped n-dodecane (FY20 milestone)• Piloted-ignition spray experiments with select fuels• Pyrolyzing sprays of doped n-dodecane with additional fuels• Ignition/soot experiments for select MCCI Co-Optima fuels

Summary



DFI	<ol style="list-style-type: none">1. Successfully conducted the world's first DFI experiments in an engine.2. DFI with only 25 vol% of an oxygenated fuel can:<ul style="list-style-type: none">• Attenuate soot incandescence by ~100X without large impacts on other emissions or efficiency.• ~10X from lower soot from fuel oxygenation, ~10X from DFI.3. DFI with dilution can break the long-standing soot/NO_x trade-off:<ul style="list-style-type: none">• Renewable, oxygenated fuels & DFI could greatly improve MCCI engine-out emissions ("zero" soot, very low NO_x, lower net CO₂) & maintain efficiency.• Provides a market "pull" for renewable fuels while maintaining compatibility with current commercial diesel fuels.4. Further effort is required to ensure MCCI surrogate fuels adequately match target-fuel performance in engine experiments.
Soot	<ul style="list-style-type: none">• Novel experimental approaches are being developed and leveraged to reveal key insights into soot formation in high-pressure sprays relevant to MCCI.• Experimental results will inform the development of an empirical model dependent on YSI, cetane number, and other parameters to provide a robust soot metric for MCCI operation.